CCR
Center for Computing Research

Kokkos: Manycore Programmability and Performance Portability

SIAM Parallel Processing
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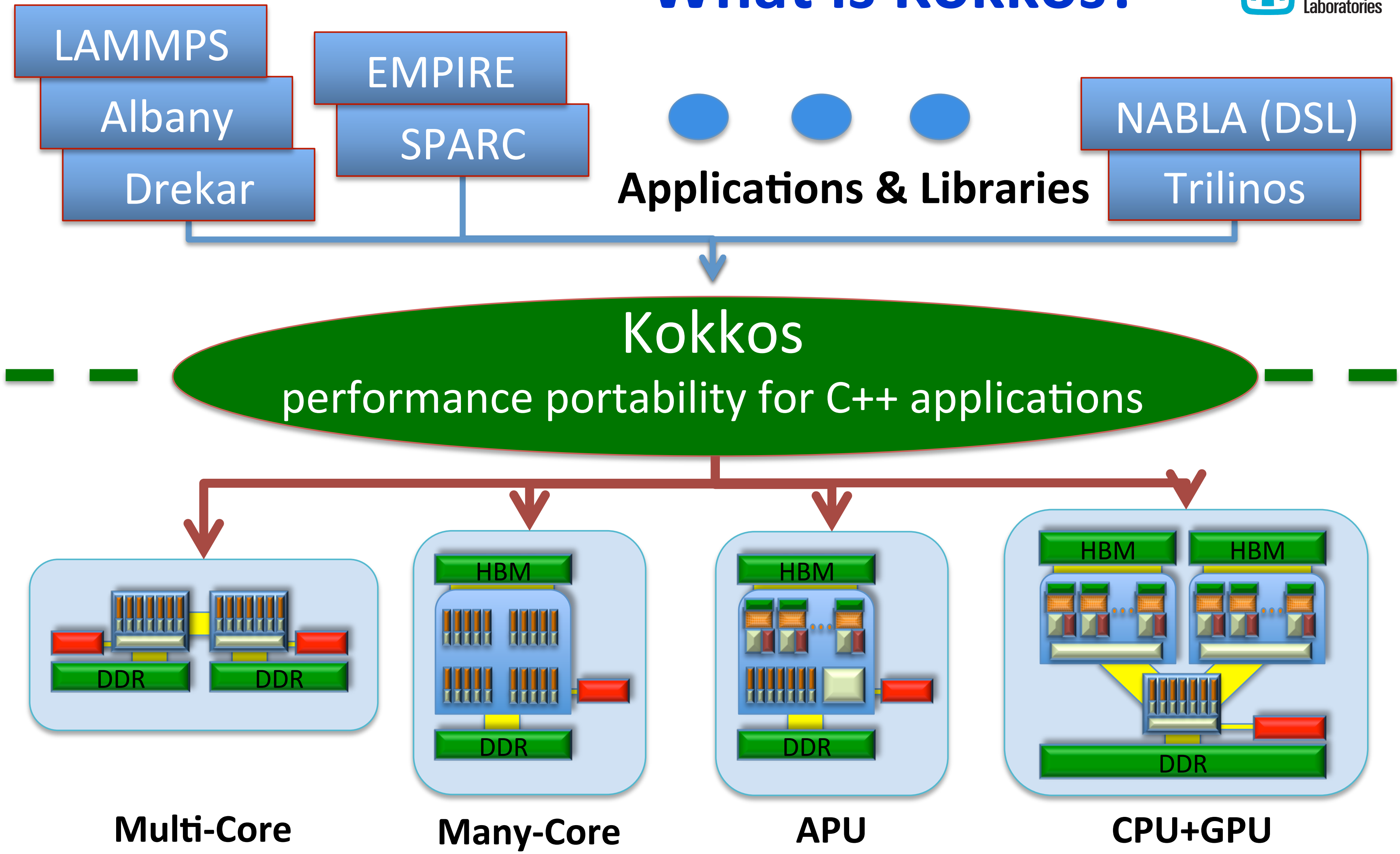
What is Kokkos?



What is *Kokkos*?

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- **κόκκος** (Greek, not an acronym)
  - Translation: "granule" or "grain" ; *like grains of sand on a beach*
- **Performance Portable Thread-Parallel Programming Model**
  - E.g., "X" in "MPI+X" ; **not** a distributed-memory programming model
  - Application identifies its parallelizable grains of computations *and* data
  - Kokkos maps those computations onto cores *and* that data onto memory
- **Fully Performance Portable C++11 Library Implementation**
  - ***Not* a language extension (e.g., OpenMP, OpenACC, OpenCL, …)**
  - **Production** – open source at https://github.com/kokkos/kokkos
  - ✓ **Multicore CPU** - including NUMA architectural concerns
  - ✓ **Intel Xeon Phi (KNC)** – toward DOE's Trinity (ATS-1) supercomputer
  - ✓ **NVIDIA GPU (Kepler)** – toward DOE's Sierra (ATS-2) supercomputer
  - ✧ **IBM Power 8** – toward DOE's Sierra (ATS-2) supercomputer
  - ✧ **AMD Fusion** – back-end in collaboration with AMD via HCC
    - **https://bitbucket.org/multicoreware/hcc/wiki/Home**

✓ Regularly tested
✧ Ramping up testing

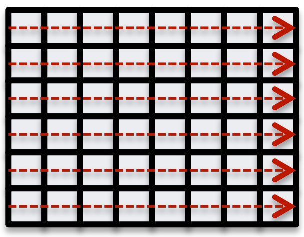
Abstractions: Patterns, Policies, and Spaces

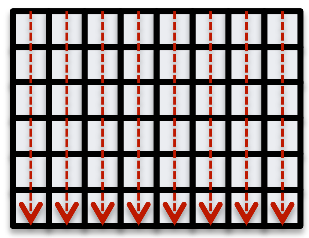
- **<u>Parallel Pattern</u> of user's computations**
  - **parallel_for, parallel_reduce, parallel_scan, task-graph, ... *(extensible)***
- **<u>Execution Policy</u> tells *how* user computation will be executed**
  - **Static scheduling, dynamic scheduling, thread-teams, ... *(extensible)***
- **<u>Execution Space</u> tells *where* user computations will execute**
  - **Which cores, numa region, GPU, ... *(extensible)***
- **<u>Memory Space</u> tells *where* user data resides**
  - **Host memory, GPU memory, high bandwidth memory, ... *(extensible)***
- **<u>Layout</u> (policy) tells *how* user data is laid out in memory**
  - **Row-major, column-major, array-of-struct, struct-of-array ... *(extensible)***
- **Differentiating: Layout and Memory Space**
  - **Versus other programming models (OpenMP, OpenACC, ...)**
  - **Critical for performance portability ...**

Layout Abstraction: Multidimensional Array

- **Classical (50 years!) data pattern for science & engineering codes**
  - Computer languages hard-wire multidimensional array <u>layout</u> mapping
  - Problem: different architectures *require* different layouts for performance
  - ➢ **Leads to architecture-specific versions of code to obtain performance**
  - E.g., "Array of Structure" ↔ "Structure of Array" redesigns

e.g.,
"row-major"
CPU caching





e.g.,
"column-major"
GPU coalescing

- **Kokkos *separates* layout from user's computational code**
  - *Choose* layout for architecture-specific memory access pattern
    - ➢ **Without modifying user's computational code**
  - **Polymorphic** layout via C++ template meta-programming *(extensible)*
    - ➢ **e.g., Hierarchical Tiling layout** (array of structure of array)
- **Bonus: easy/transparent use of special data access hardware**
  - Atomic operations, GPU texture cache, ... *(extensible)*

Performance Impact of Data Layout

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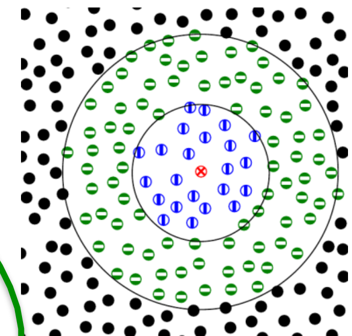
- **Molecular dynamics computational kernel in miniMD**
- **Simple Lennard Jones force model:**

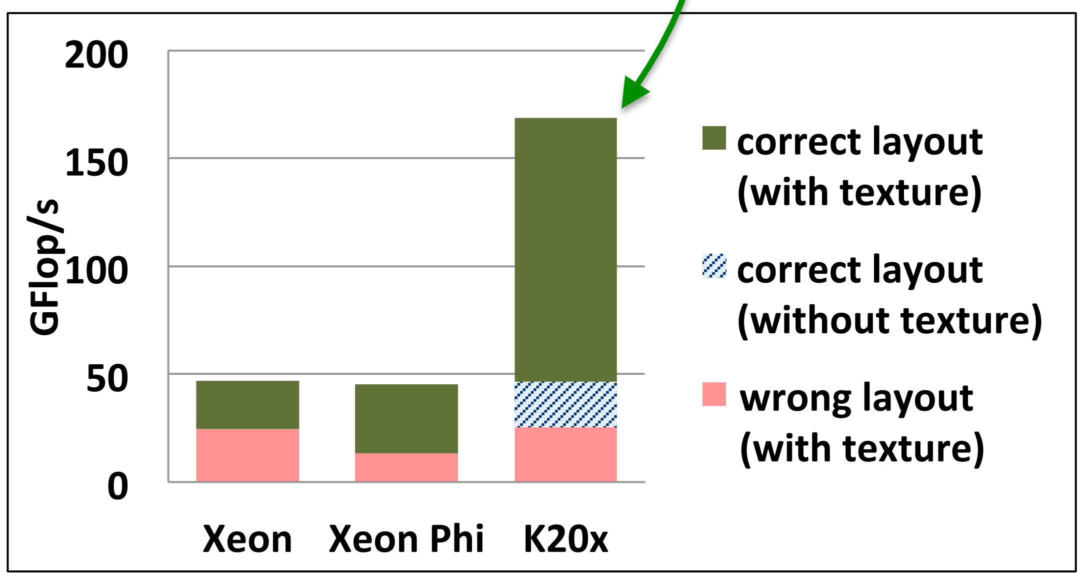
$$F_i = \sum_{j,\, r_{ij} < r_{cut}} 6\varepsilon \left[\left(\frac{\varsigma}{r_{ij}}\right)^7 - 2\left(\frac{\varsigma}{r_{ij}}\right)^{13} \right]$$

- **Atom neighbor list to avoid N^2 computations**

```
pos_i = pos(i);
for( jj = 0; jj < num_neighbors(i); jj++) {
  j = neighbors(i,jj);
  r_ij = pos(i,0..2) - pos(j,0..2); // random read 3 floats
  if (|r_ij| < r_cut) f_i += 6*e*((s/r_ij)^7 - 2*(s/r_ij)^13)
}
f(i) = f_i;
```



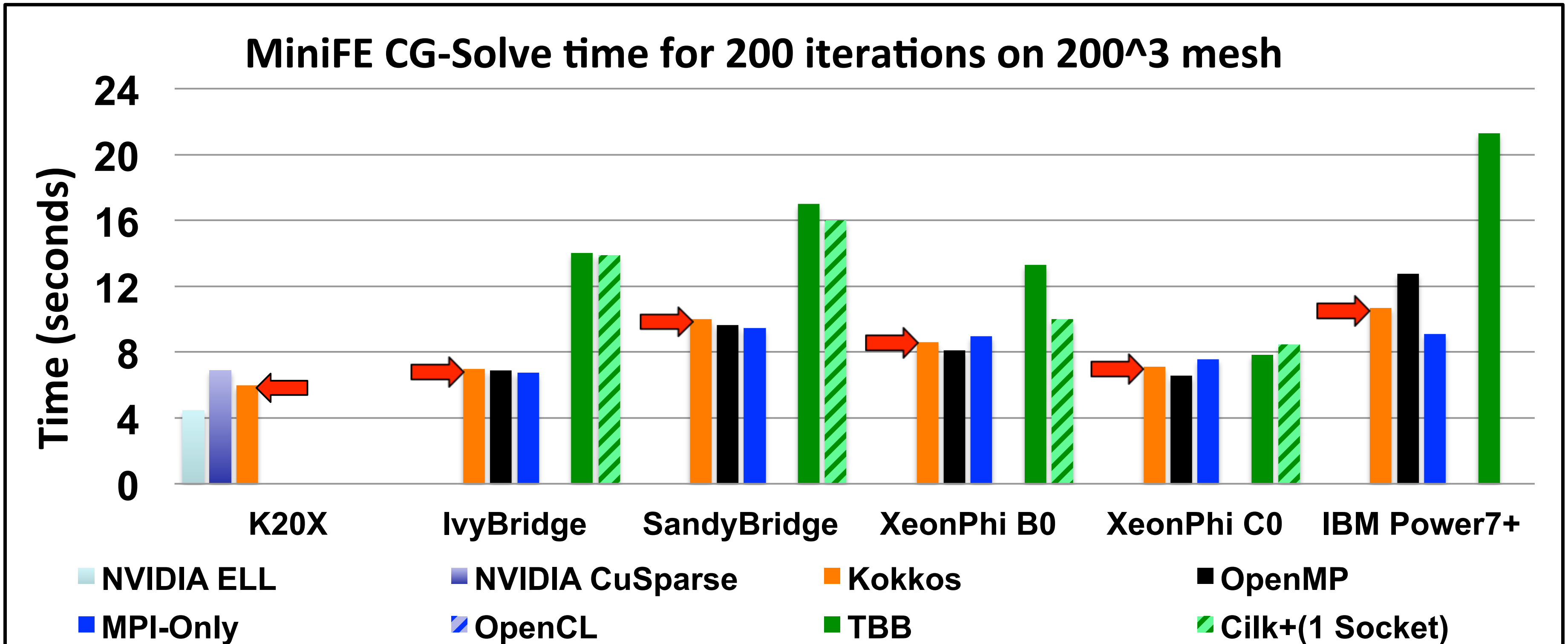
- **Test Problem**
  - 864k atoms, ~77 neighbors
  - 2D neighbor array
  - Different layouts CPU vs GPU
  - Random read 'pos' through GPU texture cache
- **Large performance loss with wrong data layout**



Performance Overhead?

Kokkos is competitive with other programming models

- Regularly performance-test mini-applications on Sandia's ASC/CSSE test beds
- MiniFE: finite element linear system iterative solver mini-app
  - Compare to versions with architecture-specialized programming models



Performance Portability & Future Proofing

Integrated mapping of users' parallel computations *and* data through abstractions of patterns, policies, spaces, *and* layout.

- **Versus other thread parallel programming models (mechanisms)**
  - OpenMP, OpenACC, OpenCL, ... have parallel execution
  - OpenMP 4 finally has execution spaces; when memory spaces ??
  - ➢ **All of these neglect data layout mapping**
    - Requiring significant code refactoring to change data access patterns
    - Cannot provide *performance* portability
  - ➢ **All require language and compiler changes for extension**
- **Kokkos extensibility "future proofing" wrt evolving architectures**
  - Library extensions, not compiler extensions
  - E.g., Intel KNL high bandwidth memory ← just another memory space
- **Productivity versus other programming models?**

Patterns, Policies, and C++11 Lambdas

- **Pattern composed with policy drives the computational body**

```
for ( int i = 0 ; i < N ; ++i ) { /* body */ }
pattern     policy                body
parallel_for ( N , [=]( int i ) { /* body */ } );
```

C++11 lambda

- **C++11 lambda implements computational body**
  - C++ compiler creates a *closure* for you: function body + captured data
    - Old school: tedium of writing a C++ class with operator()(int i)
  - Kokkos executes your closure according to pattern and policy
- **C++17 lambda within a class member function: [=,*this]**
  - Fixed defect in C++11: no way to capture *this *by value*
- **Data parallel patterns: for, reduce, scan**
- **Execution policies: range and hierarchical thread team**
- **Illustrate with the following examples…**

Example: Sparse Matrix-Vector Multiply (SPMV)

- **Baseline serial version**

```
for ( int i = 0 ; i < nrow ; ++i ) {
  for ( int j = irow[i] ; j < irow[i+1] ; ++j )
    y[i] += A[j] * x[ jcol[j] ];
}
```

- **Simple Kokkos parallel version**

```
parallel_for( nrow , KOKKOS_LAMBDA( int i ) {
  for ( int j = irow[i] ; j < irow[i+1] ; ++j )
    y[i] += A[j] * x[ jcol[j] ];
});
```

- **"nrow" implies a *Range* execution policy**
  - Call body with i = [0..nrow), call in parallel with no ordering guarantees
  - Call body in the *default* execution space
- **`KOKKOS_LAMBDA` for GPU/CUDA portability**
  - CPU : `#define KOKKOS_LAMBDA [=] /* nothing */`
  - GPU : `#define KOKKOS_LAMBDA [=] __host__ __device__`
  - GPU requires CUDA 7.5 and lambda capture-by-value [=]

Example: Dot-product and Prefix-Sum

- **Baseline serial versions,** is the pattern obvious?

```
double result = 0 ;
for ( int i = 0 ; i < N ; ++i ) { result += x[i] * y[i]; }

y[i] = 0 ;
for ( int i = 0 ; i < N ; ++i ) { y[i+i] = y[i] + x[i]; }
```

- **Simple Kokkos parallel versions**

```
parallel_reduce( N, KOKKOS_LAMBDA( int i, double & tmp ){
  tmp += x[i] * y[i] ;
}, result );

y[i] = 0 ;
parallel_scan( N, KOKKOS_LAMBDA( int i, int & tmp, bool final ){
  tmp += x[i];
  if ( final ) y[i+1] = tmp ;
});
```

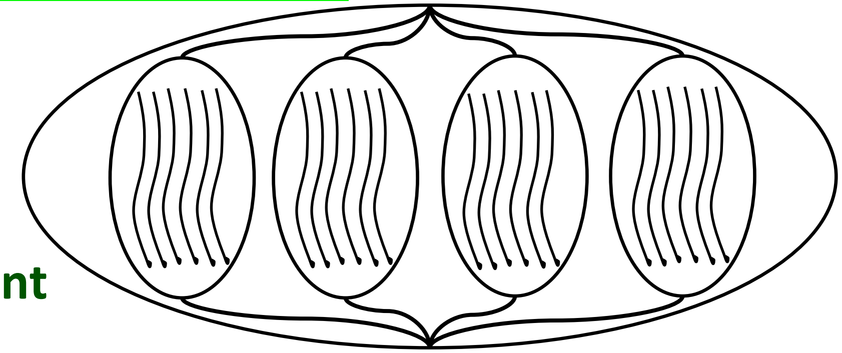
- **Kokkos manages for you:**
  - Thread local temporary variables
  - Inter-thread synchronizations and reductions of thread local temporaries

Example: Sparse Matrix-Vector Multiply (SPMV)

- **Explicit Range execution policy version**

```
parallel_for( RangePolicy<Space>(0,nrow), KOKKOS_LAMBDA(int i){
  for ( int j = irow[i] ; j < irow[i+1] ; ++j )
    y[i] += A[j] * x[ jcol[j] ];
});
```

- **Is [0 .. nrow) enough parallelism?**
  - **With O(1000)s GPU threads? That nested loop could also be parallel …**
- **Hierarchical Thread Team execution policy**
  - **`TeamPolicy<Space>(LeagueSize,TeamSize)`**
  - **OpenMP : league of teams of threads**
  - **CUDA : grid of blocks of threads**
  - **Threads within a team are concurrent**
  - **Teams within a league are not concurrent**



Example: Sparse Matrix-Vector Multiply (SPMV)

```
parallel_for( TeamPolicy<Space>(nrow,AUTO),
  KOKKOS_LAMBDA( TeamPolicy<Space>::member_type member ) {
    const int i = member.league_rank();
    double result = 0 ;
    parallel_reduce(
      TeamThreadRange(member,irow[i],irow[i+1]),
      [&]( int j , double & tmp) { tmp += A[j] * x[jcol[j]];},
      result );
    if ( member.team_rank() == 0 ) y[i] = result ;
});
```

- **Outer level of parallel pattern + execution policy**
  - **TeamPolicy requires closure (lambda) with 'member_type' argument**
    - ***member* is a handle for *thread* within s *team* within a *league***
  - **Requires KOKKOS_LAMBDA macro (CPU→GPU)**
- **Inner level of parallel pattern + execution policy**
  - **TeamThreadRange identifies *member* threads that participate**
  - **Ordinary (unmarked) C++11 lambda may be used**

Data Placement and Layout: Views

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- View< double**[3][8] , $Space_{opt}$ > a("a",N,M);
  - Allocate array data in a memory Space with dimensions [N][M][3][8]
  - *View* semantics analogous to C++11 std::shared_ptr
- a(i,j,k,l) : User's access to array datum
  - Multi-index mapping according to layout
  - "Space" accessibility enforced; e.g., GPU code cannot access CPU memory
  - Optional array bounds checking of indices for debugging
- View< ArrayType , $Layout_{opt}$, $Space_{opt}$, $Attributes_{opt}$ >
  - Explicitly declare array *layout* instead of letting Kokkos choose
  - Access intent *attributes*; e.g., atomic, random access (GPU texture cache)
- Array subview of array view
  - b = subview(a , *{10,100}* , *{200,300}* , *2* , *3*); // ranges and indices
  - View of same data, with the appropriate layout and multi-index map
- View-like functionality on-track for C++20

Thread Safety and Atomic Operations

- Some algorithms have inherent thread safety challenges
  - Histogram summing into buckets
  - Finite element assembly of linear system coefficients
  - Scatter-add pattern : `A[ index[i] ] += f( x[i] , y[i] , … );`
- Strategies for thread safety
  - *Coloring* (partitioning) of work into disjoint subsets avoids conflicts
    - Serial execution across subsets, parallel execution within a subset
    - Performance concerns: reduced parallelism and coloring algorithm overhead
  - *Atomic* operations serializes conflicts
    - Special hardware for "+=" of numeric types, perhaps reduced performance
    - Simpler to use than coloring, no loss of parallelism
- Atomics, C++11, and Kokkos
  - C++11 has "hard wired" atomic types with atomic operations
  - Kokkos provides atomic operations on ordinary types
  - C++20 atomic operations for non-atomic types is "in the works"

Other Features (new or in-development)

- **Back-ends for new & changing node architectures**
  - AMD Fusion with new open source HCC compiler
  - Intel KNL heterogeneous memory (high bandwidth memory)
  - NVIDIA GPU register shuffle for intra- thread team collectives
- **Patterns, policies, spaces, layout**
  - Dynamic scheduling (work stealing) execution policies
  - Multidimensional range policies (parallel "loop collapse")
  - Dynamically resizable arrays - thread-scalable within parallel operations
  - Directed acyclic graph (DAG) of "fine grain" tasks execution pattern/policy
  - Tiling layout mapping
- **Portable embedded performance instrumentation**
  - Selective instrumentation of individual parallel dispatch
    - parallel_for, parallel_reduce, parallel_scan

Conclusion / Takeaways

- **Performance Portability, for C++ Applications**
  - **Integrated mapping of applications' computations *and* data**
    - **Other programming models fail to map data and limit performance portability**
  - **Future proofing via designed-in extensibility and ongoing R&D**
  - **Production on Multicore CPU, Intel Xeon Phi, IBM Power 8, and NVIDIA GPU; *AMD Fusion in progress***
    - **github.com/kokkos/kokkos**
- **Productivity, for C++ Applications**
  - **C++11 lambda for simple conversion of 'for' loops to 'parallel_*pattern*'**
  - **Reduce and Scan inter-thread complexity managed by Kokkos**
  - **Hierarchical parallelism using nested patterns can increase parallelism**
- **Goal: ISO/C++ 2020 Standard subsumes Kokkos abstractions**

NOTE: SIAM-PP16, MS81, Friday 4:50pm
Performance and Productivity of Abstract C++ Programming Model